

beta-Aminobutyric acid  
541-48-0 | DTXSID4040975

Model Performance

Model	Data
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Weighted KNN model

5-fold CV (75%)		Training (75%)		Test (25%)	
Q2	RMSE	R2	RMSE	R2	RMSE
0.84	0.55	0.85	0.53	0.83	0.64

Model Results

Predicted value: 4.32

Global applicability domain: Inside

Local applicability domain index: 3.75e-01

Confidence level: 7.62e-01

Nearest Neighbors from the Training Set

<div>Image not found</div> <div>Phenylphosphinic acid</div> <div>Measured: 6.03</div> <div>Predicted: 4.42</div>	<div>Image not found</div> <div>2,2-Dimethylpropanoic acid</div> <div>Measured: 2.29</div> <div>Predicted: 2.74</div>	<div>Image not found</div> <div>Benzoic acid, 4-(methylamino)-</div> <div>Measured: 2.40</div> <div>Predicted: 4.00</div>
<div>Image not found</div> <div>3-Nitrobenzoic acid</div> <div>Measured: 7.08</div> <div>Predicted: 3.63</div>	<div>Image not found</div> <div>Dalapon-sodium</div> <div>Measured: 7.24</div> <div>Predicted: 5.61</div>	